Phonon Scattering by Line Defects

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The lattice dynamics of a solid containing small density-of-line defects has been discussed in the lattice model of Montroll and Potts. The lattice is assumed to be simple cubic. Changes in the mass and force constants along and perpendicular to the line defect are considered. The line-defect symmetry has been exploited for simplifying the phonon-scattering T matrix. The symmetry configuration in which the line defect moves gives rise to different types of local and resonance modes in two host–line-defect systems. In systems of type I, $\epsilon - \xi = 0$, where ϵ and ξ denote the relative changes in mass and force constants along the line defect, respectively. In such systems, incomplete bands of acoustic localized modes and scattering resonances occur. The lowest localized mode lies at zero frequency, whereas the lowest resonance mode occurs at a higher frequency depending upon the perturbation parameters. The widths of these incomplete bands depend upon the strength of the perturbation. At low temperatures, resonance modes might not influence the usual phonon scattering. In a more general type of solid (systems of type II), the perturbation on the line, $\epsilon - \xi$, does not vanish. Complete bands of localized and resonance acoustic modes appear in these systems. The lowest localized or resonance mode occurs at zero frequency. Resonance phonon scattering will be observed in type-II systems. The contribution of the phonon-resonance scattering by line defects in a solid is about 20% at temperatures of the order of $10^{-2}\Theta$, if there exists resonance scattering due to dislocation motion of the kind treated by Granato. Direct observation of resonance scattering by line defects is possible in bcc metals because there is no dislocation motion in these solids. The specific heat of a solid containing a small density of dislocations has been calculated. It consists of two terms: one linear and one cubic in the temperature. The linear term dominates at quite low temperatures ($T < 0.2\,^{\circ}\mathrm{K}$), whereas the cubic term is accessible to observation only in highly deformed solids.

I. INTRODUCTION

The problem of the scattering of phonons or electrons by line defects, e.g., dislocations in solids, has drawn the attention of a number of workers.[1–7] The existence of phonon-bound (or localized) states associated with a line or plane defect of isotopes was shown by Kobori[2] using Green's-function method. A number of theories put forward to determine the contribution of the dislocations to the resistivity (thermal or electrical) use the first-order perturbation theory – i.e., the Born approximation. For a review of the earlier attempts the reader is referred to the articles by Brown.[5,6] The problem of the scattering of lattice waves by the long-range static-strain field of dislocations has been treated by Ohashi[8] using a Green's-function method. He obtained magnitudes of phonon scattering which were in better agreement with the experimental results[9–11] than were those calculated by Klemens[12] and Carruthers.[13] However, in his treatment he used the Born approximation, in which the possibility of the occurrence of resonance modes is ruled out.

The existence of the phonon and electron-bound states and the scattering resonances has been shown, in general, by Brown[5] for the case of line defects. He has also discussed the resonance scattering[6] due to a screw dislocation, assuming a δ-function perturbation for the defect. The large magnitude of the dislocation thermal resistivity observed in a number of systems, such as impurities in alkali halides or Cu-Al alloys[14] can be accounted for very well by the resonance scattering mechanism. The observation of a much smaller contribution of dislocations to the thermal resistivity of some systems, such as Cu-Zn alloys[15,16] or Cu-As alloys,[15] was explained by Brown on the assumption that the scattering resonances in such systems fall, for some reason, fairly well into the subbands, and thus do not influence the energies of interest at low temperatures. The present investigations were carried out to see if there was any possibility of the existence of such high-energy scattering resonances in some particular systems.

In the present paper, the lattice dynamics of a solid having simple-cubic structure and containing a small density of parallel line defects (see Sec. II) is investigated in detail. The lattice-dynamical model of Montroll and Potts has been used in order to consider the problem. The realistic and physical nature of the results obtained on the basis of this lattice model in an analogous case of point defects has already been established in an earlier paper.[17] The perturbation due to a screw dislocation is approximated by a line defect which has a D_4 point-group symmetry. The changes in the mass and force constants along and perpendicular to the line defect are considered in writing the per-

turbation matrix. A very special case (i.e., $\beta = 0$, where β denotes the relative change in the force constant normal to the line defect) has been considered by Litzman and Cely[7] for determining the occurrence of the localized modes. We have obtained explicit expressions for determining the localized modes and scattering resonances for various irreducible representations. The Debye approximation, which is suitable for treating the long-wavelength phonons, has been used for the numerical evaluation of the Green's functions.

The possibility of the occurrence of two types of phonon scattering in Γ_1 irreducible representation which involves the motion of the line defect is seen. In Sec. III A, systems of type I in which $\epsilon - \xi = 0$, where ϵ and ξ are the relative changes in mass and force constants, respectively, along the line defect are discussed. Some incomplete bands of acoustic localized and resonance modes may appear in such systems. The incomplete band of the localized modes has its bottom at zero frequency and its width depends upon the perturbation determined by the parameters ϵ and β. The bottom of the incomplete band of the scattering resonances does not lie near zero frequency but instead lies at high frequency determined by ϵ and β. At low temperatures these resonances are not likely to be excited, and the magnitude of phonon scattering in systems of type I will be small. In Sec. III B, systems of type II in which $\epsilon - \xi \neq 0$ are discussed. In this case, complete bands of acoustic localized modes and scattering resonances occur. The bottoms of these bands lie at zero frequency and therefore resonance-phonon scattering will be observed in general. This case has been discussed by Brown.[5] The relaxation times have been determined for the two types of phonon scattering in Secs. IV A and IV B, respectively. The relaxation rate has a ω^3 dependence (ω is the phonon frequency) in the case of ordinary phonon scattering and a ω^{-1} dependence for the resonance scattering. The expressions for the specific heat of a solid containing small density-of-line defects have been obtained for both types of systems as is shown in Secs. IV A and IV B, respectively. The specific heat consists of two terms. The first term is linear in temperature, while the second term is cubic. The linear term is accessible to observation only at quite low temperatures ($T < 0.5\,^\circ$K). The expressions for the specific heat in the systems of types I and II are similar in nature. In Sec. V, the general applicability of the line-defect model to the dislocations is discussed. A detailed comparison between the predictions of the line-defect model and the fluttering model of Granato[18] has been made. Favorable conditions for observing the contributions of line defects to the thermal resistivity and specific heat have been envisaged. Comment is made upon the limitations of the scalar model.

II. LATTICE DYNAMICS

The details of the lattice dynamics of a crystal in the lattice model of Montroll and Potts can be found in an earlier paper.[19] For a lattice containing a defect, the time-independent equation of motion is given by

$$(\omega^2 \underset{\approx}{I} - \underset{\approx}{\Phi}) \underset{\sim}{U} = 0, \tag{1}$$

where $\underset{\approx}{\Phi} = \underset{\approx}{\Phi}_0 + \underset{\approx}{P}$, and $\underset{\approx}{\Phi}_0$ is the mass-reduced dynamical matrix of the perfect solid and P is the mass-reduced perturbation matrix due to the defect. $\underset{\sim}{U}$ is the atomic displacement vector of the imperfect lattice. The eigenvectors of the matrix $\underset{\approx}{\Phi}_0$ are the plane waves with dispersion relation

$$\omega_{\vec{k}}^2 = \eta \left[Z - \textstyle\sum_{\vec{n}} e^{i\vec{k}\cdot\vec{n}} \right], \tag{2}$$

where η is the mass-reduced force constant between two nearest-neighbor atoms of mass M, the $\vec{n}$ denotes the lattice position of the atom, Z is the number of nearest neighbors of an atom, and $\vec{k}$ is the wave vector of the plane wave. At low frequencies we have, in the Debye approximation,

$$\omega_k^2 = \eta a^2 k^2 = v_0^2 k^2, \tag{3}$$

where v_0 is the velocity of the long-wavelength phonons.

In the case of a line defect along the z axis the translational symmetry of the solid is retained along this direction and, therefore, one may obtain Fourier transforms with respect to z axis. The solutions of Eq. (1) may, thus, be labeled by $\vec{k}_3$, the z component of the wave vector $\vec{k}$. One may write $\vec{k} = \vec{k}_* + \vec{k}_3$, where $\vec{k}_*$ denotes the wave vector in the $k_1 k_2$ plane. The solutions of Eq. (1) are

$$\underset{\sim}{U}^{\vec{k}_3}(\vec{n}) = \underset{\sim}{y}^{\vec{k}_3}(\vec{n}_*) e^{i\vec{k}_3 \cdot \vec{n}_3}, \tag{4}$$

where $\vec{n} = \vec{n}_* + \vec{n}_3$.

The outgoing-wave solutions of Eq. (1) may be written as

$$\underset{\sim}{y}^{\vec{k}_3} = \underset{\sim}{y}_0^{\vec{k}_3} - \underset{\approx}{G}^{+} \underset{\approx}{\Delta} \underset{\sim}{y}^{\vec{k}_3}, \tag{5}$$

where $\underset{\sim}{y}_0^{\vec{k}_3}$ is the vector for the pure lattice. $\underset{\approx}{G}^{+}$ is the asymptotic value of the Fourier-transformed Green's-function matrix $\underset{\approx}{G}$ whose elements are given by

$$G(\vec{n}_* - \vec{n}_*') = \frac{\Omega_*}{(2\pi)^2} \iint \frac{e^{i\vec{k}_* \cdot (\vec{n}_* - \vec{n}_*')}}{\omega_k^2 - z} \, d\vec{k}_*, \tag{6}$$

where Ω_* is the area of the unit cell in the $\vec{k}_*$ plane and $z = \omega^2 + iO = \omega^{2+}$. The integration is over the sub-

band $\vec{k}_3$, whose bottom lies at the squared frequency $\omega_{k_3}^2$ and whose width is 8η.

The matrix elements of the Fourier transform of the perturbation matrix $\underset{\sim}{\Lambda}$ are given by

$$\Lambda(\vec{n}_*, \vec{n}_*') = \sum_{\vec{n}_3 - \vec{n}_3'} P(\vec{n}_*, \vec{n}_*', \vec{n}_3 - \vec{n}_3') e^{-i\vec{k}_3 \cdot (\vec{n}_3 - \vec{n}_3')} . \tag{7}$$

Equation (5) may be rewritten as

$$\underset{\sim}{v}^{\vec{k}_3} = \underset{\sim}{v}_0^{\vec{k}_3} - \underset{\sim}{G}^+ \underset{\sim}{T} \underset{\sim}{v}_0^{\vec{k}_3} , \tag{8}$$

where the phonon scattering T matrix is defined by

$$\underset{\sim}{T} = \underset{\sim}{\Lambda} (\underset{\sim}{I} + \underset{\sim}{G} \underset{\sim}{\Lambda})^{-1} . \tag{9}$$

For a line defect possessing some symmetry, the appropriate symmetry coordinates pertaining to the point group of the perturbation may be used to simplify the T matrix as

$$\langle \vec{q}_* | \underset{\sim}{T} | \vec{k}_* \rangle = \sum_\nu \langle \vec{q}_* | \underset{\sim}{T}_\nu | \vec{k}_* \rangle , \tag{10}$$

where the sum is over all the irreducible representations ν, $\vec{k}_*$ and $\vec{q}_*$ denote, respectively, the wave vectors of the incident and scattered plane waves in a plane normal to the line defect. $\underset{\sim}{T}_\nu$, the projected T matrix in the νth irreducible representation, is determined by

$$\langle \vec{q}_* | \underline{T}_\nu | \vec{k}_* \rangle = \frac{1}{D_\nu} \sum_{\vec{n}_*, \vec{n}_*'; \vec{n}_*''} \Lambda_{\nu, \vec{n}_*', \vec{n}_*''} Q_{\nu, \vec{n}_*'', \vec{n}_*'} \times \sum_i C_{\nu i}^*(\vec{k}_*, \vec{n}_*) C_{\nu i}(\vec{q}_*, \vec{n}_*'), \tag{11}$$

where $Q_{\nu, \vec{n}_*'', \vec{n}_*'}$ are the elements of the matrix Q defined by

$$\underline{T}_\nu = (1/D_\nu) \underline{Q}_\nu . \tag{12}$$

The $C_{\nu i}(\vec{k}_*, \vec{n}_*)$ are the symmetrized combinations of the plane waves belonging to the ith row of the νth irreducible representation and are given by

$$C_{\nu i}(\vec{k}_*, \vec{n}_*) = \frac{\Omega_*^{1/2}}{2\pi} \sum_{\vec{n}_*} U(\nu_i, \vec{n}_*) e^{i\vec{k}_* \cdot \vec{n}_*} , \tag{13}$$

where $\vec{U}(\nu_i, \vec{n}_*)$ are the coefficients of the plane wave at lattice site $\vec{n}_*$ in the symmetrized combination corresponding to the ith row of the νth irreducible representation.

The asymptotic value of the Green's function for $\vec{n}_* \gg \vec{n}_*'$ is given by (see Appendix)

$$G^+(\vec{n}_* - \vec{n}_*') = \frac{e^{i\pi/4} e^{ik_* n_*} e^{-i\vec{q}_* \cdot \vec{n}_*'}}{2\eta (2\pi k_* n_*)^{1/2}} . \tag{14}$$

Using Eqs. (10), (11), (13), and (14), Eq. (8) may be rewritten as

$$v^{\vec{k}_3}(\vec{n}_*) = v_0^{\vec{k}_3}(\vec{n}_*) - \frac{(2\pi)^2 e^{i\pi/4}}{2\Omega_* \eta (2\pi k_*)^{1/2}} \times \sum_\nu \langle \vec{q}_* | T_\nu | \vec{k}_* \rangle \frac{v_0^{\vec{k}_3}(\vec{n}_*)}{n_*^{1/2}} . \tag{15}$$

The scattering amplitude may thus be expressed as

$$f(\vec{q}_*, \vec{k}_*) = \sum_\nu f_\nu(\vec{q}_*, \vec{k}_*), \tag{16}$$

where the contribution of the νth irreducible representation is given by

$$f_\nu(\vec{q}_*, \vec{k}_*) = \frac{-(2\pi)^{3/2} e^{i\pi/4}}{2 v_0^2 k_*^{1/2}} \langle \vec{q}_* | T_\nu | \vec{k}_* \rangle . \tag{17}$$

If the problem is discussed in terms of the phase shifts of the partial waves, the scattering amplitude of a plane wave of wave vector $\vec{k}_*$, scattered by a cylindrically symmetric potential, is given by

$$f(\theta) = \frac{2e^{i\pi/4}}{(2\pi k_*)^{1/2}} \sum_{m=-\infty}^{+\infty} e^{i\delta_m} \sin\delta_m \, e^{im\theta} , \tag{18}$$

where δ_m is the phase shift of the mth partial radial wave, and θ is the angle between the wave vector of the incoming wave and a vector to the point of observation.

III. LINE-DEFECT MODEL

A simple-cubic lattice having a line defect along the z axis is now considered. The line defect is made up of atoms of masses $(M + \Delta M)$ which interact with their nearest neighbors with a set of changed force constants as shown in Fig. 1. The matrix elements of the perturbation matrix are given by

$$\Lambda(\vec{0}, \vec{0}) = -\epsilon\omega^2 + 4\alpha + 2\gamma(1 - \cos k_3 a) = \delta ,$$

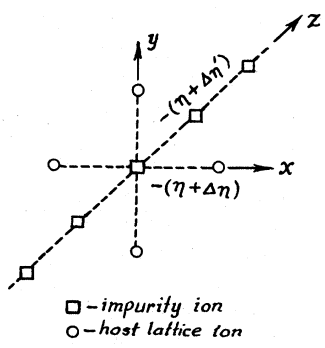

FIG. 1. Line-defect model.

$$\Lambda(\vec{0},\vec{\Delta}_x)=\Lambda(\vec{0},\vec{\Delta}_y)=-\alpha,$$
$$\Lambda(\vec{\Delta}_x,\vec{\Delta}_x)=\Lambda(\vec{\Delta}_y,\vec{\Delta}_y)=\alpha, \tag{19}$$

where

$$\vec{\Delta}_x=(\pm 1,0) \quad \text{and} \quad \vec{\Delta}_y=(0,\pm 1);$$

$$\epsilon=\Delta M/M, \quad \alpha=\Delta\eta/M, \quad \gamma=\Delta\eta'/M.$$

The η' and η are the changes in the force constants in directions along and perpendicular to the line defect.

The point-group symmetry of the line defect is D_4. The symmetry coordinates belonging to the various irreducible representations occurring in the problem are presented in Table I.

The projected matrix elements are

$$\langle\Gamma_1|\underline{\Lambda}(\omega^2)|\Gamma_1\rangle=\begin{pmatrix}\delta & -2\alpha\\ -2\alpha & \alpha\end{pmatrix},$$
$$\langle\Gamma_3|\underline{\Lambda}(\omega^2)|\Gamma_3\rangle=\alpha, \tag{20}$$
$$\langle\Gamma_5|\underline{\Lambda}(\omega^2)|\Gamma_5\rangle=\alpha.$$

The projected matrix elements of the Green's-function matrix are

$$\langle\Gamma_1|\underline{G}(z)|\Gamma_1\rangle=\begin{pmatrix}G_0 & 2G_1\\ 2G_1 & G_s\end{pmatrix},$$
$$\langle\Gamma_5|\underline{G}(z)|\Gamma_5\rangle=G_0-G_2, \tag{21}$$

and

$$\langle\Gamma_3|\underline{G}(z)|\Gamma_3\rangle=G_0+G_2-2G_3,$$

where

$$G_0=G(00), \quad G_1=G(10), \quad G_2=G(20), \quad G_3=G(11),$$
$$G_s=G_0+G_2+2G_3.$$

TABLE I. Normalized symmetry coordinates corresponding to the various irreducible representations.

$\vec{\Delta}$		Γ_1		Γ_5		Γ_3
0	0	1	0	0	0	0
1	0	0	$\frac{1}{2}$	$\sqrt{\frac{1}{2}}$	0	$\frac{1}{2}$
0	1	0	$\frac{1}{2}$	0	$\sqrt{\frac{1}{2}}$	$-\frac{1}{2}$
-1	0	0	$\frac{1}{2}$	$-\sqrt{\frac{1}{2}}$	0	$\frac{1}{2}$
0	-1	0	$\frac{1}{2}$	0	$-\sqrt{\frac{1}{2}}$	$-\frac{1}{2}$
Partial wave		s		p		d

The projected elements of the T matrix are, thus, given by

$$\langle\Gamma_1|\underline{T}(z)|\Gamma_1\rangle$$
$$=\frac{1}{D_{\Gamma_1}}\begin{pmatrix}\delta-4\alpha\rho(A-1)G_1 & -2\alpha(1+\rho G_1)\\ -2\alpha(1+\rho G_1) & \alpha(1+\rho G_0)\end{pmatrix}, \tag{22a}$$

where the resonance denominator D_{Γ_1} is explicitly given by

$$D_{\Gamma_1}=(1+\beta)-[(\epsilon-\beta)\omega^2+(\beta-\xi)\omega_{\vec{k}_3}^2]G_0$$
$$-\beta[(1+\epsilon)\omega^2-(1+\xi)\omega_{\vec{k}_3}^2]G_1, \tag{22b}$$
$$\langle\Gamma_5|\underline{T}(z)|\Gamma_5\rangle=\alpha[1+\alpha(G_0-G_2)]^{-1}, \tag{22c}$$

and

$$\langle\Gamma_3|\underline{T}(z)|\Gamma_3\rangle=\alpha[1+\alpha(G_0+G_2-2G_3)]^{-1}. \tag{22d}$$

Here

$$\rho=-\epsilon\omega^2+4\gamma\ \sin^2 k_3\tfrac{1}{2}a=-\epsilon\omega^2+\xi\omega_{\vec{k}_3}^2;$$
$$\beta=\alpha/\eta=\Delta\eta/\eta, \qquad \xi=\gamma/\eta=\Delta\eta'/\eta;$$
$$\omega_{\vec{k}_3}^2=4\eta\ \sin^2 k_3\tfrac{1}{2}a, \qquad A=(\omega_{\vec{k}}^2-\omega_{\vec{k}_3}^2)/4\eta. \tag{22e}$$

For simplifying the projected matrix elements of the Γ_1 irreducible representation the relations between different Green's-function matrix elements obtained from the equation of motion of the perfect lattice have been used. For the details, see an earlier paper.[20] For this particular problem these relations are

$$G_s=4(1-A)G_1$$

and

$$G_1=(1-A)G_0-(4\eta)^{-1}. \tag{23}$$

It may be easily shown[5,7] that

$$G(\vec{n}_*)=G(0)+B(\vec{n}_*), \tag{24}$$

where $B(\vec{n}_*)$ is always a finite quantity.

A. Localized States

The localized or bound modes of the symmetry motion ν, corresponding to the subband $\vec{k}_3$, are determined by

$$\mathrm{Re}D_\nu(\omega^2)=0. \tag{25}$$

For the Γ_5 and Γ_3 irreducible representations, the resonance denominators D_{Γ_5} and D_{Γ_3} involve the

following combinations of the Green's-function elements:

$(G_0 - G_2)$ in the Γ_5 irr. rep.,

$(G_0 + G_2 - 2G_3)$ in the Γ_3 irr. rep.

The real value of the Green's-function matrix element G_0 diverges at the boundaries of the subband (see Appendix), but the real values of the above combinations of the Green's-function elements are always finite due to a property of the Green's-function elements given by Eq. (24). As a result, the occurrence of the localized modes in the irreducible representations Γ_5 and Γ_3 depends upon the strength of the perturbation denoted by α (force-constant change normal to the line defect). This behavior is similar to the case of point-defect scattering.

The equation for the determination of the acoustic localized modes in Γ_1 irreducible representation may be written as

$$(1+\beta)+(\beta/4\eta)[(\epsilon-\xi)\omega_{k_3}^2-(1+\epsilon)\Delta] - \left\{\left[1+\beta+\beta\left(\frac{\Delta}{4\eta}\right)\right] \times[(\epsilon-\xi)\omega_{k_3}^2-\epsilon\Delta]-\beta\frac{\Delta^2}{4\eta}\right\}\mathrm{Re}G_0(\omega^2)=0, \quad (26)$$

where $\Delta=\omega_{k_3}^2-\omega_L^2$ denotes the depth of the localized mode below the bottom of the subband $\vec{k}_3$. If the analytical value of G_0 evaluated in the Debye approximation is used (see Appendix), the equation may be rewritten as

$$(1+\beta)+\left(\frac{\beta}{4\eta}\right)[(\epsilon-\xi)\omega_{k_3}^2-(1+\epsilon)\Delta] - \left(\frac{1}{4\eta\pi}\right)\left\{(1+\beta)(\epsilon-\xi)\omega_{k_3}^2+\left[\beta(\epsilon-\xi)\left(\frac{\omega_{k_3}^2}{4\eta}\right) - \epsilon(1+\beta)\right]\Delta-\beta(1+\epsilon)\left(\frac{\Delta^2}{4\eta}\right)\right\}\ln\Delta/(8\eta-\Delta)=0 . \quad (27)$$

The coefficient of the logarithmic term within the curly brackets consists of three terms: The first is independent of Δ, while the remaining two are dependent on Δ. Now, two different types of defect-host systems shall be considered.

Systems of type I. If it happens that $\epsilon-\xi=0$, Eq. (27) is further simplified to

$$(1+\beta)-\beta(1+\epsilon)\frac{\Delta}{4\eta}+\pi^{-1}\left[(1+\beta)\epsilon+\beta(1+\epsilon)\left(\frac{\Delta}{4\eta}\right)\right] \times\left(\frac{\Delta}{4\eta}\right)\ln\left(\frac{\Delta}{(8\eta-\Delta)}\right)=0 . \quad (28)$$

This equation may be solved numerically for a given set of parameters ϵ and β. The positive solutions of Δ, if they exist, will give rise to localized modes. The equation will not admit infinitely small solution as is clear from the following considerations: For example, if it is assumed that there exist solutions of Eq. (28) such that $\Delta \to 0^+$, then these solutions must satisfy the following approximate condition:

$$1+(\epsilon/\pi)(\Delta/4\eta)\ln(\Delta/4\eta)=0 . \quad (29)$$

The second term of this equation tends to zero as $\Delta \to 0^+$. Consequently, infinitely small Δ will not satisfy the above condition and local acoustic modes will not appear very near to the lower boundary of a subband.

In order to see the appearance of finite solutions of Eq. (28), an example was considered. Suppose there was interest in the solutions lying at a depth η below the bottom of a subband, then the relation should hold

$$1+0.75\beta=0.5(\beta+0.3)\epsilon . \quad (30)$$

Since the lowest physical value of β is -1, the left-hand side of Eq. (30) is always positive. This leads to the choice of two sets of perturbation parameters

$$\epsilon<0, \quad \beta<-0.3$$

or

$$\epsilon>0, \quad \beta>-0.3 .$$

A few sets of parameters which satisfy Eq. (30) are shown in Table II. It is observed that, in real solids, the local acoustic mode of a subband will occur at $\Delta=\eta$, for positive values of ϵ and β only.

It is obvious that the solutions of Eq. (28) are true for any of the subbands. Also, there is only one bound state for each subband. The lowest local mode at zero frequency occurs for a subband whose bottom lies at $\Delta_1(\Delta_1<4\eta)$, which is the existing solution of Eq. (28). The uppermost local mode appears due to a subband whose lower boundary lies at 4η. Thus, in systems of type I, an incomplete band of local acoustic modes appears. The lower and upper boundaries of this band lie at $\omega^2=0$, and

TABLE II. Values of the perturbation parameters ϵ and β which lead to the occurrence of acoustic localized modes at a depth η below the bottom of a subband, in terms of the frequency (squared).

β	ϵ
-0.8	- 1.6
-0.5	- 6.0
-0.2	-17.0
1.0	3.0
1.7	2.3

at $\omega^2 = 4\eta - \Delta_1$, as shown in Fig. 2. It may be noted that this band lies within the original band of the pure solid. The frequency spectrum in this band is similar to that for a one-dimensional chain of atoms.

Systems of type II. For these systems, $\epsilon - \xi$ does not vanish. As a result, a term independent of Δ, e.g., $(\epsilon - \xi)\omega_{k_3}^2$, is always present as a coefficient of the Green's function $G_0(\Delta)$. The real part of $G_0(\Delta)$ diverges as $\Delta \to 0^+$ and, consequently, an infinitely small solution of Eq. (26) always appears for a set of realistic values of ϵ, ξ, and β. A local mode appears very near to the lower boundary of each subband $\vec{k}_3$. Thus, the existence of a complete band of local acoustic modes whose lower and upper boundaries lie at $\omega^2 = 0$ and 4η, respectively, is observed. This is shown in Fig. 3 and is similar to that for a linear chain of atoms. It should be noted that the solutions of Eq. (26) now depend on the subband, in contrast to that for the systems of type I. For a particular case, $\beta = 0$, Litzman and Cely[7] have predicted the occurrence of a complete band of local acoustic modes and an incomplete band of local optical modes.

B. Resonance Modes

The arguments similar to that of the case of localized modes hold good for the appearance of the acoustic resonance modes of Γ_5 and Γ_3 irreducible representations. The scattering resonances appear only for a certain strength of the perturbation parameter α. In the case of Γ_1 irreducible representation, the acoustic resonance modes are determined by

$$(1+\beta)+\frac{\beta}{4\eta}\left[(\epsilon-\xi)\omega_{k_3}^2+(1+\epsilon)\Delta\right]$$
$$+\frac{1}{4\eta\pi}\Bigg\{(1+\beta)(\epsilon\omega^2-\xi\,\omega_{k_3}^2)$$
$$-\left[\beta(\epsilon-\xi)\omega_{k_3}^2-\epsilon(1+\beta)\right]\Delta$$
$$-\beta(1+\epsilon)\frac{\Delta^2}{4\eta}\Bigg\}\ln\frac{\Delta}{8\eta-\Delta}=0, \tag{31}$$

where, $\Delta = \omega_R^2 - \omega_{k_3}^2$, and it denotes the height of the scattering resonance ω_R above the bottom of the subband $\vec{k}_3$.

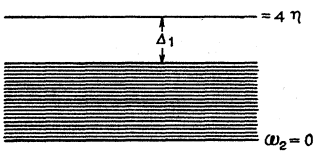

FIG. 2. Incomplete band of localized acoustic modes appearing in systems of type I; Δ_1 is the positive solution of Eq. (28).

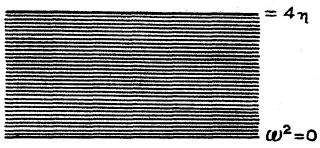

FIG. 3. Complete band of the localized or resonance acoustic modes which appear in systems of type II.

The half-width of the scattering resonance is determined by

$$\frac{\Gamma}{2}=\left[\mathrm{Im}D_{\Gamma_1}(z)\Big/\frac{d}{d\omega^2}\,\mathrm{Re}D_{\Gamma_1}(z)\right]_{\omega_R},$$

where

$$\mathrm{Im}D_{\Gamma_1}(z)=-\{(1+\beta)(\epsilon-\xi)\omega_{k_3}^2$$
$$+[\epsilon(1+\beta)-\beta(\epsilon-\xi)\omega_{k_3}^2/4\eta]\Delta-\beta(1+\epsilon)\Delta^2/4\eta\}, \tag{32a}$$

and

$$\frac{d}{d\omega^2}\mathrm{Re}D_{\Gamma_1}(z)=\beta(1+\epsilon)+\pi^{-1}\left(\epsilon(1+\beta)-\beta(\epsilon-\xi)\frac{\omega_{k_3}^2}{4\eta}\right.$$
$$\left.-2\beta(1+\epsilon)\frac{\Delta}{4\eta}\right)\ln\frac{\Delta}{8\eta-\Delta}+\pi^{-1}\Bigg[(1+\beta)(\epsilon-\xi)\omega_{k_3}^2$$
$$+\left(\epsilon(1+\beta)-\beta(\epsilon-\xi)\frac{\omega_{k_3}^2}{4\eta}\right)\Delta-\beta(1+\epsilon)\frac{\Delta^2}{4\eta}\Bigg]\frac{8\eta}{(8\eta-\Delta)}. \tag{32b}$$

Now two cases similar to that of the localized modes may be discussed.

For systems of type I, where $(\epsilon - \xi)\omega_{k_3}^2 = 0$, Eq. (31) is reduced to a simple form

$$(1+\beta)+\beta(1+\epsilon)\frac{\Delta}{4\eta}+\pi^{-1}\left(\epsilon(1+\beta)-\beta(1+\epsilon)\frac{\Delta}{4\eta}\right)$$
$$\times\left(\frac{\Delta}{4\eta}\ln\frac{\Delta}{8\eta-\Delta}\right)=0. \tag{33}$$

Again, due to the presence of the logarithmic term

$$(\Delta/4\eta)\ln[\Delta/(8\eta-\Delta)],$$

which diverges as $\Delta \to 0$, scattering resonances will not appear very near the bottom of the subband. For the case of resonances appearing at a distance η from the bottom of the subband, the parameters ϵ and β should satisfy the condition

$$1+\tfrac{5}{4}\beta-\epsilon/2\pi+\beta\epsilon/8=0$$

or

$$\beta=-8(1-\epsilon/2\pi)/(10+\epsilon)\ . \tag{34}$$

For a physical value of $\epsilon<2\pi$, a negative β will give rise to these resonances. A few values of the parameters ϵ, β together with the corresponding linewidths (at half maximum) of the scattering resonances which are at a height η above the bottom of the subband, are presented in Table III. It may be noted that the widths of the scattering resonances are small for low values of ϵ but are large for high values of ϵ. For realistic values of ϵ, the half-width of the scattering resonance is of the order of 0.5η, which is half of its distance from the bottom. Further, we note that the half-widths have positive values and, therefore, these appear in systems of type-I as resonances, in contrast to the systems of type II where antiresonances appear.

Thus, it may be concluded that in the systems of type I, the scattering resonances do not appear very close to the bottom of the subband. An incomplete band of acoustic resonance modes appears, whose bottom lies at high frequencies Δ_2, which are determined by the parameters ϵ and β. The width of these resonances are of the order of their frequencies. This incomplete band is shown in Fig. 4.

For the systems of type II, where $(\epsilon-\xi)\omega_{k_3}^2\neq 0$, similar to that of the case of localized modes, the scattering resonances lie very close to the bottom of the subband and a complete band of the acoustic-resonance modes will appear irrespective of the strength of the perturbation. This case is shown in Fig. 3. The half-widths of these scattering resonances are given by

$$\tfrac{1}{2}\Gamma=-\pi\Delta\ . \tag{35}$$

These values are negative and, therefore, the scattering resonances are, in fact, antiresonances.

IV. SCATTERING AMPLITUDE AND SPECIFIC HEAT

In Sec. III, two types of the host-defect-line systems were discussed. In the systems of type I,

TABLE III. Values of the parameters ϵ and β and the corresponding half-widths which lead to the occurrence of acoustic scattering resonances at a height η above the bottom of a subband.

$\epsilon=\xi$	β	$\frac{1}{2}\Gamma$
0	-0.8	0.2η
1	-0.6	0.45η
3	-0.3	η
6	0	3η

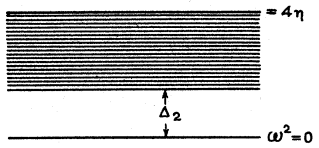

FIG. 4. Incomplete band of scattering resonance states appearing in systems of type I; Δ_2 is the solution of Eq. (31).

where $\epsilon-\xi=0$, incomplete bands of localized modes and scattering resonances appear. These resonances occur at high frequencies and their widths are not an appreciable fraction of the total width, 8η, of a subband. The scattering resonances, thus, do not influence the scattering of the long-wavelength phonons which are predominant at low temperatures. The resonance scattering mechanism will not be observed in such systems. In the systems of type II, resonance scattering occurs. The transport and thermodynamic properties of these systems are expected to be different owing to the difference in the nature of the phonon scattering which occurs in the system, and each will be treated separately.

In order to calculate the scattering amplitude and changes in the density of states, a phase shift δ_ν for the νth irreducible representation is defined,

$$\tan\delta_\nu=-\mathrm{Im}D_\nu/\mathrm{Re}D_\nu\ . \tag{36}$$

The symmetrized contributions of the plane waves belonging to the irreducible representations Γ_1, Γ_3, and Γ_5 correspond to the s, p, and d partial radial waves, respectively. The expressions for the phase shifts for these waves may easily be written down after using Eqs. (22).

A. Systems of Type I

In the absence of resonance scattering, which is likely to occur in the systems of type I, it is safe to limit ourselves to the first order of the wave vector in order to determine the small phase shifts.

For the s-type Γ_1 irreducible representation, to first order in $\vec{k}_*$,

$$\mathrm{Im}D_{\Gamma_1}=-(1+\beta)\epsilon\,\frac{\Delta}{4\eta}\ ,$$

and

$$\mathrm{Re}D_{\Gamma_1}=(1+\beta)\left(1+\frac{\epsilon}{\pi}\,\frac{\Delta}{4\eta}\,\ln\frac{\Delta}{8\eta}\right)\ .$$

In the limit $\Delta\to 0$,

$$\delta_{\Gamma_1}=\delta_s=\epsilon\,\Delta/4\eta$$
$$=\tfrac{1}{4}\epsilon a^2k_*^2\ . \tag{37}$$

In the case of p-type Γ_5 irreducible representation, we have

$$\mathrm{Im}D_{\Gamma_5} = \tfrac{1}{4}\beta a^2 k_*^2$$

and

$$\mathrm{Re}D_{\Gamma_5} = 1 + \alpha \mathrm{Re}(G_0 - G_2)$$

$$= 1 + K\beta \text{ (say)},$$

where

$$K = \eta\,[\mathrm{Re}(G_0 - G_2)]_{\Delta=0}$$

is a numerical constant. For simple-cubic lattice, the value of K has been evaluated numerically in the Debye approximation and is seen to be 0.3. The phase shift of the p type is given by

$$\delta_{\Gamma_5} = \delta_p = \beta a^2 k_*^2/4(1+K\beta)\ . \tag{38}$$

The phase shift of the d-type Γ_3 irreducible representation is seen to be of the order of k_*^4 and it is ignored in a first-order calculation.

1. *Relaxation Time*

To first order in k_*, the total scattering amplitude is given by

$$f(\theta) = [2e^{i\pi/4}/(2\pi k_*)^{1/2}]\,(\delta_s + 2\delta_p \cos\theta)\ . \tag{39}$$

The differential scattering cross section is determined by

$$\frac{d\sigma}{dA} = |f(\theta)|^2\ .$$

The total scattering width Q is, thus, given by

$$Q = \int_0^{2\pi} \frac{d\sigma}{dA}\,(1-\cos\theta)\,d\theta$$

$$= \tfrac{1}{8}a^4 k_*^3\,[(\epsilon + 2\beta/(1+K\beta))^2 + \epsilon^2]\ . \tag{40}$$

The relaxation rate may be written as

$$\tau^{-1}(k_*) = v_0 L^{-1} = c v_0 Q/a^2\ , \tag{41}$$

where c is the concentration of the parallel dislocations and is equal to $a^2\sigma$ for unit volume of the solid. The σ denotes the density of the line defects. Thus, for the relaxation time we have

$$\tau^{-1}(k_*) = \tfrac{1}{8}v_0\sigma\,[(\epsilon + 2\beta/(1+K\beta))^2 + \epsilon^2]\,k_*^3\ . \tag{42}$$

This relaxation rate has an expected ω^3 dependence.

2. *Specific Heat*

The change in the density of states, i.e., the fraction of the states lying between the frequencies Δ and $\Delta + d\Delta$ in the νth irreducible representation, for a subband is determined by

$$\hat{\delta}N_\nu = \frac{g_\nu}{N_* \pi}\,\frac{d\delta_\nu}{d\Delta} = \frac{g_\nu}{\pi N_* v_0^2}\,\frac{d\delta_\nu}{dk_*^2}\ , \tag{43}$$

where N_* is the total number of states lying in the subband $\vec{k}_3$.

The total change in the density of states due to a density of dislocations σ is given by

$$\hat{\delta}N = \frac{\sigma a^2}{\pi v_0^2}\,\frac{d}{dk_*^2}\,(\delta_s + 2\delta_p)$$

$$= \frac{\sigma a^2}{4\pi\eta}\left(\epsilon - \frac{2\beta}{1+K\beta}\right)\ . \tag{44}$$

Since the density of states in the subband of the pure lattice is given by $N_0 = (4\pi\eta)^{-1}$, the total change in the density of states may be rewritten as

$$\hat{\delta}N = \sigma a^2 N_0\,[\epsilon - 2\beta/(1+K\beta)]\ . \tag{45}$$

The total density of states in a subband is, thus, given by

$$N = N_0\,\{1 + \sigma a^2[\epsilon - 2\beta/(1+K\beta)]\}\ . \tag{46}$$

It may be noted that the density of states in a subband of the imperfect lattice is independent of the location of the subband and, therefore, one may easily calculate the specific heat of the solid containing dislocations by adding the contributions of all subbands whose bottoms lie between the squared frequencies 0 and 4η. Thus, it may be written for the specific heat

$$C_v(\sigma) = \sum_{\text{all subbands}} N(\sigma) = C_v(0)\left[1 + \sigma a^2\left(\epsilon - \frac{2\beta}{1+K\beta}\right)\right]\ . \tag{47}$$

In addition to the specific heat given by the Eq. (47), there is an extra contribution due to the incomplete acoustic band of the localized modes, if it exists. The density of these localized modes is similar to that of the density of states of phonons of a one-dimensional lattice. Therefore, the contribution of these localized modes has a linear temperature dependence and has a negligible magnitude[7] as compared to the T^3-dependent specific heat of a solid at moderately low temperatures ($T > 1\ ^\circ$K). However, at very low temperatures ($T < 0.5\ ^\circ$K), the linear term has an appreciable contribution and it may dominate over the cubic term (see Sec. V).

B. Systems of Type II

In general, for these systems we see an appearance of the scattering resonances in Γ_1 irreducible representation. The phase shifts in this irreducible representation are large, and they are given by

$$\tan\delta_{\Gamma_1} = \frac{(1+\beta)(\epsilon-\xi)(\omega_{k_3}^2/4\eta)}{(1+\beta)+\beta(\epsilon-\xi)(\omega_{k_3}^2/4\eta)+(1+\beta)(\epsilon-\xi)(\omega_{k_3}^2/4\eta)\ln(\Delta/8\eta)} . \tag{48}$$

If the resonance occurs at $\Delta=\Delta_0$, Eq. (48) may be written in the form

$$\tan\delta_{\Gamma_1} = -\Gamma/2(\Delta-\Delta_0) , \tag{49}$$

where $\frac{1}{2}\Gamma$, the half-width of the scattering resonance, is given by Eq. (35). Thus,

$$\sin^2\delta_{\Gamma_1} = \frac{\frac{1}{2}\Gamma}{(\Delta-\Delta_0)^2+(\frac{1}{2}\Gamma)^2} , \tag{50}$$

From Eq. (50), it is seen that as $\Delta\to\Delta_0$,

$$\delta_{\Gamma_1}\to\tfrac{1}{2}\pi \quad \text{and} \quad \sin^2\delta_{\Gamma_1}\to 1 . \tag{51}$$

Now, a scattering resonance occurs at a very small value of $\Delta(=\Delta_0)$ and the width of the resonance, which is of the order of $2\pi\Delta_0$, is very small. Therefore, a majority of the modes in a subband will not be influenced by the scattering resonance and will be normally scattered. For such modes in the low-lying subbands, i.e., for small values of $\omega_{k_3}^2$ and Δ,

$$\tan\delta_{\Gamma_1} = \delta_{\Gamma_1} = (1/4\eta)[(\epsilon-\xi)\omega_{k_3}^2+\epsilon\Delta] . \tag{52}$$

For the case of Γ_5 irreducible representation, the phase shift is similar to an expression as given by Eq. (38).

1. *Relaxation Time*

Since the magnitude of the resonance scattering is much larger than the ordinary phonon scattering, only the resonance scattering of Γ_1 irreducible representation is considered for determining the relaxation rate. The scattering amplitude for the resonance scattering of the s partial wave may be expressed as

$$f(\theta) = -2e^{-i\pi/4}/(2\pi k_*)^{1/2} . \tag{53}$$

The total scattering width Q is, thus, given by

$$Q = 4k_*^{-1} . \tag{54}$$

The relaxation rate has a simple form

$$\tau^{-1}(k_*) = 4\sigma v_0 k_*^{-1} . \tag{55}$$

This relaxation rate has a ω^{-1} dependence.

Brown[5] has shown that in the case of alkali halides the experimental values of the relaxation rates give rise to those values of $\sin^2\delta$ which are quite close to unity. In the case of Cu-Zn and Cu-As alloys the values of $\sin^2\delta$ are seen to be small, which shows the nonexistence of the resonance scattering in these systems.

2. *Specific Heat*

The change in the density of states in Γ_1 irreducible representation due to the occurrence of antiresonance at Δ_0 is given by

$$\hat{\delta}N_{\Gamma_1} = (\Gamma/2\pi N_*)[(\Delta-\Delta_0)^2+\tfrac{1}{4}\Gamma^2]^{-1} . \tag{56}$$

In order to determine the total change in the number of states due to the finite width of the antiresonance, the above expression should be integrated between the limits 0 to $\Delta_0+\frac{1}{2}\Gamma$. Thus, for finding the change in the number of states it is necessary to evaluate

$$\int_0^{\Delta_0+\Gamma/2}\hat{\delta}N_{\Gamma_1}\,d\Delta = 0.35\Gamma/|\Gamma| = -0.35. \tag{57}$$

This value differs from unity, which was the value obtained by Brown, who replaced the limits of integration by $\pm\infty$ in conformity to his assumption that the integral converges fairly rapidly – which, in fact, is not true, because of the slow convergence of the integrand.

There is a net decrease of 0.35 in the number of states for each subband. The density of these subbands is similar to that of a one-dimensional lattice because of the relation $\omega_{k_3}^2 = 4\eta\sin^2 k_3\frac{1}{2}a$. But a complete band of acoustic localized modes is also present and, therefore, there is a net increase of 0.65 in the number of states of the one-dimensional band. The contribution of this band to the specific heat has a linear temperature dependence and is given by

$$C_1 \simeq \pi^2 N k\sigma a^2(kT/\hbar\omega_{1D}) , \tag{58}$$

where ω_{1D} is the Debye frequency of a one-dimensional lattice.

In addition to the above linear temperature-dependent contribution of Γ_1 irreducible representation, there is another contribution to the specific heat made by those low-lying modes of the subband, which lie far away from the scattering resonance. For these modes, to first order in squared frequency, the phase shift is obtained by

$$\delta_s = (1/4\eta)(\epsilon\omega^2 - \xi\omega_{k_3}^2) . \tag{59}$$

The change in the number of states is given by

$$\hat{\delta}N_{\Gamma_1} = \frac{\sigma a^2}{4\pi v_0^2}\frac{d\delta_s}{dk_*^2} = \frac{\sigma a^2 \epsilon}{4\pi\eta} . \tag{60}$$

This expression is similar to that of $\hat{\delta}N_{\Gamma_1}$ calculated for the systems of type I. The density of states in Γ_3 irreducible representation, which is not affected by the scattering resonances of Γ_1 irreducible representation, is similar to that of systems of type I. Therefore, the total change in the number of states of the subband is represented by an expression which is exactly identical to the systems of type I. The contribution of these states to the specific heat is given by Eq. (47), which shows a T^3 dependence. The linear temperature-dependent contribution obtained above may be ignored in comparison to a large T^3-dependent contribution to the specific heat of a solid at moderately low temperatures ($T > 1$ °K). But at low enough temperatures ($T < 0.2$ °K) the linear term may dominate as has already been observed by Granato[18] when he considered a similar linear temperature-dependent contribution due to the fluttering modes of a moving dislocation.

V. DISCUSSION

The general applicability of the line-defect model to the dislocations in real solids is now considered. Granato[18] has proposed a model in which resonance-phonon scattering from dislocations takes place. He considers "fluttering" of a segment of a dislocation line pinned at both ends and the resulting resonance scattering of phonons from these fluttering modes which are similar to the standing waves in a stretched string. In the formulation, a continuum elastic theory was used and the dislocation core effects were completely neglected. In considering phonon scattering from the line defects, dislocation core effects are treated, neglecting the effect of the long-range strain field around the dislocation.

In the thermal conductivity measurements of the real solids, a combined effect of the two different resonance scattering mechanisms was observed as mentioned above. In Granato's model, the mean free path l_f is, approximately, given by[18]

$$l_f(\omega) = (\omega/2\pi^2 C\sigma)[\ln(\Theta/5T)]^2 , \tag{61}$$

where C is the velocity of the fluttering modes and Θ is the Debye temperature. This mean free path has a slowly varying logarithimic temperature dependence. For $T = 10^{-2}\Theta$, $l_f(\omega)$ may be written as

$$l_f(\omega) = 0.4\,(C\sigma)^{-1}\omega . \tag{62}$$

In case of the systems of type II, where one observes the resonance-phonon scattering, the mean free path l_c can be written as [see Eq. (55)]

$$l_c(\omega) = (4v_0\sigma)^{-1}\omega, \tag{63}$$

where v_0 is the phonon velocity in the pure solid. To compare the two mean free paths, it is noted that for typical metals, $p = v_0/C \approx 2.5$. Thus, at temperatures of the order of $10^{-2}\Theta$, the contribution of the line defects is about 20% of the total scattering. At higher temperatures, the contribution will be still larger. The frequency dependence is the same for both types of resonance scattering but their magnitudes are different. In the usual range of the measurements, the temperature dependence of the thermal conductivity in the fluttering model[18] is T^n, where n lies between 3.3 and 3.5. The thermal conductivity depends on T^4 in the line-defect model. The detection of this small difference in the predictions of the two theories seems to be difficult.

In the systems of type I, where the line-defect model gives rise to the normal phonon scattering, we may observe only the resonance scattering by the dislocation motion, if it exists. In the systems of type II, we expect a combined effect of the two scattering mechanisms.

The resonance scattering of the phonons from the fluttering modes occurs if the dislocations are free to move in crystals. The dislocation motion has been predicted in alkali halides and fcc metals after measuring the changes in the elastic constants because of the dislocations.[21,22] By measuring the amplitude-dependent internal friction, Chambers[21] has shown that the dislocations are free to move at low temperatures in fcc metals like Al and Cu, but not in bcc metals like Ta, Nb, Mo, and W. Bauer and Gordon,[22] after measuring the changes in Young's modulus have shown that the dislocations are mobile in alkali halides and that they can be pinned by x irradiation at low temperatures. The thermal conductivity measurements on deformed alkali halides have shown a large magnitude of phonon scattering. This fact supports the existence of the resonance scattering from the dislocations. On the other hand, a fcc metal like Cu should show the resonance scattering, but the thermal-conductivity measurements made by Kemp *et al.*[15] and

Lomer *et al.*[16] on Cu-Zn and Cu-As alloys do not show such an effect. However, Charsley and Salter[14] have observed a high resistivity due to the dislocations in Cu-Al alloys. Kusunoki and Suzuki[23] have postulated the existence of the resonance scattering from the vibrating-edge dislocations in Cottrell atmosphere in order to explain the large lattice thermal conductivity observed in Cu-Al alloys in the temperature range 1.6–4.2 °K. Unfortunately, there are no experimental data available about bcc crystals which might show the occurrence of the resonance-phonon scattering from the line defects because there is no dislocation motion in these solids. A systematic experimental work is very much needed to understand the general occurrence of the resonance-phonon scattering in the solids.

The evidence for the temperature dependence of the thermal conductivity predicted by the resonance scattering is provided by some experimental measurements on the superconductors. In the measurements on superconducting lead below 1 °K by Felix *et al.*,[24] a conductivity of the form $AT^{3.7\pm0.2}$ has been observed, where the values of A for three specimens lie between 0.1 and 0.2 for the temperature range 0.15–0.8 °K. In superconducting indium, Graham[25] has observed a T^4-dependent conductivity in the temperature range 0.2–1 °K. It may be noted that there are no other mechanisms which predict such a large temperature dependence and still require a suitable dislocation density ($\sim 2\times10^8$ cm^{-2}) to produce the right order of magnitude of the phonon scattering. The frequency dependence of the relaxation rates ranging from ω^0 to ω^2 have been observed in alkali halides[9–11] or metals[14–16,26] in contrast to a ω^{-1} dependence predicted by the resonance scattering. A temperature-independent thermal conductivity due to the dislocation dipoles in alkali halides has been predicted by Gruner and Bross.[27] Again, more experimental measurements are required to clarify the present situation of the temperature dependence of the thermal conductivity in solids.

In the absence of resonance scattering in solids, the contributions made by the line-defect scattering and also by the long-range static-strain field scattering estimated earlier by a number of workers[8,12,13] would be observed. The contribution of the ω^3-dependent scattering from the line defects will be appreciable at high frequencies, and will not ordinarily be observed at low temperatures. Thus, the thermal conductivity of these solids will exhibit a T^2-dependent thermal conductivity due to the static-strain field of the dislocations. This has been observed in a number of solids.[9–11,14–16,26]

The contribution of the dislocations to the specific heat of the solids will now be considered. In Granato's model of the dislocation motion, there appears a linear temperature-dependent term given by

$$C_v^l = p(\tfrac{1}{3}\pi^2)(\sigma a^2/Z)Nk(T/\Theta)\,, \qquad (64)$$

where Z is the number of atoms per unit cell of the lattice. Assuming that for a typical solid, $p \approx 2.5$, $Z=1$ for a simple-cubic lattice, and $\Theta\,(=\hbar\omega_{1D}/k)$ is the Debye temperature of one-dimensional lattice, we observe that this contribution is nearly equal to the linear term of the line-defect model given by Eq. (58). In the systems of type II, where complete bands of local modes appear, the contributions are very nearly equal to each other. In the systems of type I, there appears a difference in magnitudes because of the occurrence of the incomplete band. The contribution of the linear term to the specific heat will be appreciable at very low temperatures ($T \approx 0.1$–0.2 °K) as has been shown by Granato.[18] At higher temperatures ($T > 1$ °K), the contribution seems to be negligible.

In addition to the linear term, the line-defect model predicts a T^3-dependent contribution given by Eq. (47). The contribution was estimated for a metal containing a density of dislocations equal to 10^{13} cm^{-2}, and it was found that its contribution to the specific heat of a pure solid is 10%. Thus, the contribution of the cubic term may be observed only in highly deformed solids where the interaction between the dislocations is not appreciable.

In the present study of the phonon scattering from the line defects, a number of assumptions and simplifications have been made which require explanation and comment.

First, a simplified lattice model, i.e., of Montroll and Potts, has been used in the calculations. But upon considering the applicability of these results to a more general lattice there is no disappointment. The occurrence of the scattering resonances or local modes in the scalar model can easily be generalized to a more realistic lattice. In Sec. III, it has been observed that these modes occur in a symmetry configuration which includes the motion of the line defect, e.g., Γ_1 irreducible representation in the scalar model. This happens because of the presence of the Green's function G_0 in Eq. (26) or (31), which determine the existence of the local or resonance mode. The function $G_0(\Delta)$ diverges to $\pm\infty$ as the incident phonon frequency approaches the boundaries of a subband from either side. If we consider a more realistic model of the lattice, such as the one discussed below, it can be seen easily that the Green's function $G_0(\Delta)$ always appears in the resonance denominator for that symmetry motion which contains the motion of the line defect. For example, this symmetry motion is E_u in the lattice considered below. It is analogous to the case of the point-defect scattering where the same thing is true for all the monatomic[28] or diatomic cubic crystals[20,29] with nearest-neighbor interactions. The two-dimensional Green's function

$G_0(\Delta)$ always diverges when the incident phonon frequency approaches the boundaries of the subband. The above arguments are also true for the case of the vector model of the lattice.

Second, the behavior of the defect systems depends upon the coefficient of $G_0(\Delta)$ in the resonance denominator of Γ_1 symmetry configuration, which involves the motion of the line defect (Δ is the separation of the local or resonance mode from the bottom of a subband). If in a more realistic lattice the Δ-independent term in the coefficient of $G_0(\Delta)$ vanishes, then infinitely small solutions of Eq. (26) or (31) will not exist because of the vanishing of the term containing $G_0(\Delta)$, as $\Delta \to 0$. Therefore, in systems of type I, incomplete bands of the local or the resonance acoustic mode will appear. On the other hand, if the Δ-independent term does not vanish, then infinitely small solutions of Eq. (26) or (31) always exist. Therefore, in systems of type II, the complete bands of the local or the resonance acoustic mode will appear. Consequently, the use of a more realistic lattice model does not alter the general features of the results obtained in the scalar model. However, one difference between the behavior of the scalar and vector model should be noted. In the scalar lattice model, we observe one local or resonance acoustic mode for each subband, which may not be true in the case of the vector model. The occurrence of these modes depends upon the detailed behavior of $G_0(\Delta)$. If there exists certain maxima or minima of G_0, inside or outside a subband, more than one solution of Eq. (26) or (31) may exist and, correspondingly, a large number of the local or resonance modes will appear for each subband. Further, if a one-band model such as has been used here is not used, more than one local or resonance mode between the two given subbands might be expected.

Regarding the numerical estimates made on the basis of the Montroll-Potts model, reference is made to an analogous case of the point-defect scattering. For the case of substitutional point defects, it has been observed that the results obtained on the basis of the scalar model are not only qualitative but also semiquantitative. The frequency and the linewidth of a low-lying resonance mode due to the presence of an weakly interacting impurity have been seen to be very realistic.[17] An estimate[30] of the force-constant changes due to impurities in a number of metals is found to be realistic. Further, the calculated phonon relaxation rates[31] due to the monovalent impurities in solids are comparable to the corresponding estimates obtained in a more realistic calculation. Therefore, one may expect that the present estimates obtained in a scalar model will not be too far from the realistic values and will be useful in finding the approximate numerical values of various physical quantities which are not readily available if one starts with a more realistic model of the crystal lattice.

Finally, comment will be made on the symmetry motions which appear in the scalar model. The symmetry motions involved in the scalar model are totally different from those appearing in a realistic lattice. A comparison between them has never been encouraging in an analogous case of the point-defect scattering. In the present case, if a vector-lattice model of displacements on the core and nearest-neighbor atoms of a (100) line defect in a simple-cubic lattice is considered, a totally different set of irreducible representations is present. The symmetry configurations, in which the line defect moves, are of odd parity $A_{2u}(\Gamma_2)$ or $E_u(\Gamma_5)$ motions in contrast to the even parity Γ_1 symmetry motion which appears in the scalar model. Thus, the symmetry motions present in the scalar model should not be taken seriously. Their use is limited to the qualitative and semiquantitative estimation of physical quantities.

The model of the line defect is nearer to a perturbation model of a screw dislocation in a solid. The case of an edge dislocation, which has an antisymmetric perturbation, is not substantially different from that of a screw dislocation.[5] Further, the choice of a simple-cubic lattice does not restrict the validity of the present results, which could easily be generalized to fcc or bcc lattices analogous to the case of point-defect scattering.[19]

VI. CONCLUSIONS

The properties of two types of the host line-defect systems have been investigated. In the systems of type I, the perturbation factor, $\epsilon - \xi$, vanishes, while in the systems of type II it does not. For the systems of type I, the incomplete bands of localized and resonance acoustic modes exist. The bottom of the incomplete band of localized modes will lie at the zero frequency and its width will depend upon the strength of the perturbation. The lowest-resonance mode does not appear at zero frequency but appears at a higher frequency. At low temperatures, when the dislocation contribution to the resistivity is appreciable, these scattering resonances due to the line defect may not be excited. No resonance scattering will be observed in type-I systems, but the phonon scattering by the long-range static-strain field will dominate and will give rise to a T^2-dependent thermal conductivity.

In the systems of type II, the existence of complete bands of the local or the resonance acoustic mode will always be observed. The lower boundaries of these bands start from the lowest frequency, i.e., $\omega = 0$. The resonance scattering will be observed in the systems of type II. The contribution of the resonance scattering due to the line

defects has been estimated and is seen to be about 25% of the contribution, if it exists, of the resonance scattering due to a vibrating dislocation segment. The direct observation of the line-defect resonance scattering will be possible in solids having bcc crystal structure where the dislocation segments are not free to move.

The contribution of a small density of dislocations to the specific heat consists of two terms. The first term, which is linear in temperature, is similar to the specific heat of a linear chain of atoms. At low temperatures ($T > 1\,^\circ$K), the linear term will be negligible but it may dominate at quite low temperatures ($T < 0.2\,^\circ$K). The second term, which is cubic in temperature, has an appreciable contribution to the specific heat only in highly deformed solids, where its effect might be masked by the interaction of dislocations among themselves.

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APPENDIX

The Green's-function matrix element for a cubic lattice is given by

$$G(\vec{n}_*) = \frac{\Omega_*}{(2\pi)^2} \iint \frac{e^{i\vec{k}_* \cdot \vec{n}_*}}{\omega_{\vec{k}}^2 - \omega^{2+}} d\vec{k}_* \,. \tag{A1}$$

For a simple-cubic lattice, we have

$$\omega_{\vec{k}}^2 = \omega_{\vec{k}_3}^2 + 2\eta(2 - \cos k_1 a - \cos k_2 a) \,,$$

where

$$\omega_{\vec{k}_3}^2 = 2\eta(1 - \cos k_3 \tfrac{1}{2} a) \,.$$

The Green's function has the explicit form

$$G(\vec{n}_*) = \left(\frac{a}{2\pi}\right)^2 \frac{1}{2\eta} \times \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} \frac{e^{(k_1 l + k_2 m) a}}{\rho - i0 - \cos k_1 a - \cos k_2 a} dk_1 dk_2 \,, \tag{A2}$$

where $\vec{n}_* = \{l,\ m\}$ and

$$\rho = 2 + (1/2\eta)(\omega_{\vec{k}_3}^2 - \omega^2) \,.$$

For $\rho > 0$, we may write Eq. (A2) in the form

$$G(\vec{n}_*) = (-i^{l+m+1}/2\eta) \int_0^\infty e^{-i\rho t} J_l(t) J_m(t)\, dt \,, \tag{A3}$$

where $J_m(t)$ is the Bessel function of the real argument of the mth order. The above integrals may be evaluated numerically. For the case of $\omega^2 < \omega_{k_3}^2$, the Green's functions are real and may be expressed as the integrals of the Bessel functions of the imaginary argument $I_m(t)$. It may be noted that these Green's-function matrix elements are independent of the location of the subband if the frequencies are measured with respect to the bottom of the subband, which lies at $\omega_{\vec{k}_3}^2$.

In order to have analytical values of the Green's functions, a Debye approximation may be used in which $\omega_{\vec{k}}^2 - \omega_{\vec{k}_3}^2 = v_0^2 k_*^2$. Equation (A2) may be written as

$$G(\vec{n}_*) = \left(\frac{a}{2\pi}\right)^2 \int_0^{k_{\max}} \int_{-\pi}^{\pi} \frac{e^{ik_* n_* \cos\theta}}{\omega_k^2 - \omega^{2+}} k_*\, dk_*\, d\theta$$

$$= \frac{a^2}{2\pi} \int_0^{k_{\max}} \frac{J_0(k_* n_*)}{\omega_k^{2+} - \omega^2} k_*\, dk_* \,, \tag{A4}$$

if one uses the integral representation of the zeroth-order Bessel function. The imaginary part is given by

$$\mathrm{Im}G(\vec{n}_*) = i\pi \frac{a^2}{2\pi} \frac{1}{2\eta a^2} \int_0^{k_{\max}} J_0(k_* n_*)\, \delta(q_*^2 - k_*^2)\, dk_*^2$$

$$= i(4\eta)^{-1} J_0(q_* n_*) \,, \tag{A5}$$

where $\omega^2 - \omega_{k_3}^2 = v_0^2 q_*^2$ is used. The real part of $G(\vec{n}_*)$ is given by

$$\mathrm{Re}G(\vec{n}_*) = \frac{1}{4\eta\pi} P \int_{\omega_{\vec{k}_3}^2}^{\omega_{\vec{k}_3}^2 + 8\eta} \frac{J_0(k_* n_*)}{\omega_k^2 - \omega^2} d\omega_k^2 \,. \tag{A6}$$

The value of this integral may easily be evaluated numerically. For $\vec{n}_* = (0,\ 0)$, the following analytical expressions are found:

$$\mathrm{Im}G_0 = i(4\eta)^{-1} \quad \text{for} \quad \omega^2 > \omega_{k_3}^2$$

and

$$\mathrm{Re}G_0 = \mp (4\eta\pi)^{-1} \ln\{|\Delta|/(8\eta - |\Delta|)\} \tag{A7}$$

for $\Delta = \omega^2 - \omega_{k_3}^2 > 0$ or < 0 .

The upper sign in Eq. (A7) is applicable to a frequency within the $\vec{k}_3$ subband and the lower one to a frequency below the lower boundary of the subband. To first order in q_*,

$$\mathrm{Im}G(\vec{n}_*) = (i/4\eta)[1 - (\tfrac{1}{2} q_* n_*)^2] \,. \tag{A8}$$

The asymptotic value of the Green's function in the

Debye approximation is determined by

$$G(\vec{n}_* - \vec{n}'_*) = \frac{a^2}{2\pi}\int_0^{k_{\max}} \frac{J_0\{k_* |\vec{n}_* - \vec{n}'_*|\}}{\omega_k^2 - \omega^{2*}} k_*\, dk_* .$$

For $(\vec{n}_* - \vec{n}'_*) \to \infty$,

$$J_0\{k_* |\vec{n}_* - \vec{n}'_*|\} = \left(\frac{2}{\pi k_* |\vec{n}_* - \vec{n}'_*|}\right)^{1/2} \times \cos\{k_* |\vec{n}_* - \vec{n}'_*| - \tfrac{1}{4}\pi\} .$$

Thus, after replacing the upper limit by ∞,

$$G^+(\vec{n}_* - \vec{n}'_*) = \frac{e^{i\pi/4} e^{ik_* n_*}}{2\eta(2\pi k_* n_*)^{1/2}}\, e^{iq_* \cdot \vec{n}'_*} , \qquad \text{(A9)}$$

where $n_* \gg n'_*$, and $\vec{q}_* = (k_*/n_*)\vec{n}_*$ is a vector of magnitude $|k_*|$ in the direction of the radius vector $\vec{n}_*$.

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Electronic Specific Heats and Superconductivity in the Group-V Transition Metals*

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Electronic specific heats of Nb-V alloys were measured from 1.5 to 14 °K and on the basis of these measurements superconductivity parameters were calculated. Both the McMillan and the Hopfield theories were used to try to understand the cause of the broad minimum in T_c with alloying composition. The McMillan theory indicates that the cause is due to a weakening of the electron-phonon interaction parameter. The Hopfield theory could not adequately predict the existence of the minimum in these alloys.

I. INTRODUCTION

The superconducting behavior of Nb-V solid-solution alloys is unusual. Whereas the superconducting transition temperatures of Nb and V are both relatively high, 9.2 and 5.5 °K, respectively, the variation of T_c in the alloys goes through a pronounced minimum at a composition of about $Nb_{0.50}V_{0.50}$. The effect cannot be correlated with Matthias's e/a factor, since both Nb and V belong to group 5. This minimum, furthermore, occurs in solid solutions of compounds in which Nb and V are the principal